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Spatial distribution of local tunneling conductivity due to interference and Coulomb interaction effects for deep and shallow impurities on semiconductor surfaces

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(Dated: May 21, 2010)

Spatial distribution of local tunneling conductivity was investigated for deep and shallow impurities on semiconductor surfaces. Non-equilibrium Coulomb interaction and interference effects were taken into account and analyzed theoretically with the help of Keldysh formalism. Two models were investigated: mean field self-consistent approach for shallow impurity state and Hubbard-I model for deep impurity state. We have found that not only above the impurity but also at the distances comparable to the lattice period both effects interference between direct and resonant tunneling channels and on-site Coulomb repulsion of localized electrons strongly modifies form of tunneling conductivity measured by the scanning tunneling microscopy/spectroscopy (STM/STS).

PACS numbers: 71.55.-i

Keywords: D. Fano resonance; D. Coulomb interaction; D. Mixed valence; D. Hubbard I; D. Impurity; D. Tunneling conductivity spatial distribution

I. INTRODUCTION

Impurity states at surface and interfaces of semiconductors strongly modify the local electronic structure and consequently determine the behavior of tunneling characteristics in STM/STS contacts [1–3]. Experimental and theoretical investigations of tunneling through impurity atom energy level in the case of multichannel transport reveal Fano-type line shape in local tunneling conductivity when STM metallic tip is positioned above the impurity [4, 6, 8]. Transformation of Fano-type line shape in local tunneling conductivity depending on distance value from impurity was also recently investigated [5, 7]. Most of the experiments are carried out with the help of scanning tunneling microscopy/spectroscopy technique [1, 8–10] and theoretical calculations usually deals with Green's functions formalism [7, 11]. Comparison between experimental STS results obtained at different distance values from the impurity [5] and theoretical investigations of single impurities influence on tunneling conductivity [7] provide information whether electron transport occurs coherently or incoherently and gives an opportunity to initialize impurity type. All these effects are caused by local changes of the initial density of states due to interactions of non-equilibrium particles in the contact area. Taking into account Coulomb interaction of conduction electrons with non-equilibrium localized charges can result in nontrivial behavior of tunneling characteristics calculated in the case of STM metallic tip positioned above the impurity atom [11–13]. However influence of Coulomb interaction effects on local tunneling conductivity measured apart from the impurity is a prob-

lem of great interest due to the possibility of impurities types initialization.

So in this work we present the modification of formula, which describe spatial distribution of local tunneling conductivity in vicinity of impurity in the case of interference between resonant and direct tunneling channels [7] due to Coulomb interaction. We performed calculations for two extreme cases when resonant tunneling takes place through deep impurity state and through shallow impurity state. We applied mean field self-consistent approach for shallow impurity state and in the case of deep impurity non-equilibrium Coulomb interaction effects were studied with the use of Hubbard-I model. Both approaches were analysed with the use of Keldysh formalism [14]. We have found that taking into account Coulomb interaction in addition to interference between tunneling channels leads to drastical changing of the tunneling conductivity form depending on the values of tunneling rates and distance from impurity.

II. THE SUGGESTED MODEL AND MAIN RESULTS

We shall analyze tunneling between semiconductor surface (1D atomic chain) and metallic STM tip for deep and shallow impurities in the presence of Coulomb interaction. The model of tunneling contact formed by semiconductor and metallic tip is depicted in Fig. 1. 1D atomic chain consists of similar atoms with energy levels ε_1 and similar tunneling transfer amplitudes \mathfrak{J} between the atoms. Distance between the atoms in the chain is the same and equal to a . Atomic chain includes impurity with energy ε_d , tunneling transitions from the impurity atom to the semiconductor and metallic tip are described by the tunneling transfer amplitudes τ and T correspondingly. Direct tunneling between the surface continuous spectrum states and tip states is described

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by the transfer amplitude t .

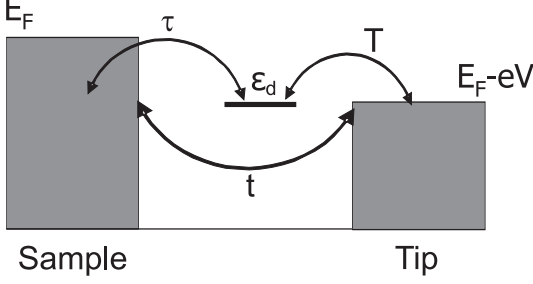


FIG. 1: Schematic diagram of direct and resonant tunneling channels.

The model system semiconductor-impurity state-metallic tip in the presence of Coulomb interaction can be described by the Hamiltonian: \hat{H} :

$$\hat{H} = \hat{H}_0 + \hat{H}_{imp} + \hat{H}_{tun} + \hat{H}_{tip}$$

$$\begin{aligned}\hat{H}_0 &= \sum_{k\sigma} \varepsilon_k c_{k\sigma}^\dagger c_{k\sigma} + \sum_{kk'\sigma} \mathfrak{I} c_{k\sigma}^\dagger c_{k'\sigma} + h.c. \\ \hat{H}_{tun} &= \sum_k \tau c_{k\sigma}^\dagger c_{d\sigma} + \sum_p T c_{d\sigma}^\dagger c_{p\sigma} + \sum_{kp} t c_{k\sigma}^\dagger c_{p\sigma} + h.c. \\ \hat{H}_{imp} &= \sum_{d\sigma} \varepsilon_d c_{d\sigma}^\dagger c_{d\sigma} + U n_{d\sigma} n_{d-\sigma}; \hat{H}_{tip} = \sum_{p\sigma} \varepsilon_p c_{p\sigma}^\dagger c_{p\sigma}\end{aligned}$$

Indices k and p label the states in the left (semiconductor) and right (tip) lead, respectively. The index d indicates that impurity electron operator is involved. U is the on-site Coulomb repulsion of localized electrons, $n_{d\sigma} = c_{d\sigma}^\dagger c_{d\sigma}$, $c_{d\sigma}$ destroys impurity electron with spin σ . \hat{H}_0 is a typical Hamiltonian for atomic chain with hoppings without any impurities. \hat{H}_{tun} describes resonant tunneling transitions from the impurity state to the semiconductor and metallic tip and direct transitions between the tunneling contact leads. \hat{H}_{imp} corresponds to the electrons in the localized state formed by the impurity atom, \hat{H}_{tip} describes conduction electrons in the metallic tip.

With the use of diagram technique for non-equilibrium processes [14] one can get expression for the spatial distribution of local tunneling conductivity without Coulomb interaction [7]:

$$\begin{aligned}\frac{dI}{dV}(\omega, x) &= \sqrt{\gamma_{kp}\gamma_{kd}\gamma_{pd}\nu_k^0} \text{Re} G_{dd}^R(\omega) \cos(2k_x(\omega)x) + \\ &+ \gamma_{kp}(\gamma_{kd} + \gamma_{pd})\nu_k^0 \text{Im} G_{dd}^R(\omega) \cos(2k_x(\omega)x) + \\ &+ \frac{\gamma_{kd}\gamma_{pd}}{\gamma_{kd} + \gamma_{pd}} \text{Im} G_{dd}^R(\omega) + \\ &+ \frac{\gamma_{kd}^2\gamma_{pd}\gamma_{kp}(\omega - \varepsilon_d) \cos(2k_x(\omega)x)}{((\omega - \varepsilon_d)^2 + (\gamma_{kd} + \gamma_{pd})^2)^2} + \\ &+ \gamma_{kp}\nu_k^0 \left(1 + \frac{(\omega - \varepsilon_d)^2 + \gamma_{kd}^2 - \gamma_{pd}(\omega - \varepsilon_d)}{(\omega - \varepsilon_d)^2 + (\gamma_{kd} + \gamma_{pd})^2}\right) \cdot \\ &\cdot \left(\frac{(\omega - \varepsilon_d)^2 + (\gamma_{kd} + \gamma_{pd})^2(1 - \cos(2k_x(\omega)x))}{(\omega - \varepsilon_d)^2 + (\gamma_{kd} + \gamma_{pd})^2} + \right. \\ &\left. + \frac{\gamma_{pd}(\gamma_{pd} + \gamma_{kd}) \cos(2k_x(\omega)x)}{(\omega - \varepsilon_d)^2 + (\gamma_{kd} + \gamma_{pd})^2}\right) \end{aligned} \quad (2)$$

where impurity retarded Green's function is defined by the expression:

$$G_{dd}^R(\omega) = \frac{1}{\omega - \varepsilon_d - i(\gamma_{kd} + \gamma_{pd})} \quad (3)$$

Relaxation rates γ_{kd} , γ_{pd} are determined by electron tunneling transitions from localized states to the leads k and p continuum states and relaxation rate γ_{kp} corresponds to direct tunneling transitions between k and p continuum states $\sum_p T^2 \text{Im} G_{pp}^{0R} = \gamma_{pd}$; $\sum_p t^2 \text{Im} G_{pp}^{0R} = \gamma_{kp}$; $\sum_k \tau^2 \text{Im} G_{kk}^{0R} = \gamma_{kd}$. ν_k^0 is unperturbed density of states in semiconductor. Expression for $k_x(\omega)$ can be found from the 1D atomic chain dispersion law:

$$\omega(k_x) = 2\mathfrak{I} \cdot \cos(k_x a) \quad (4)$$

Let us now analyze modification of formula 2 due to Coulomb interaction effects in the case of deep impurities with the help of Hubbard-I model (Hamiltonian of suggested model has the form of expression 1). Taking into account Coulomb interaction in this model leads to formation of two well separated impurity energy levels ε_d and $\varepsilon_d + U$ instead of one initial level ε_d . It is reasonable to use approximation in which the strongest interaction of the considered model - the on-site Coulomb repulsion U - is included in $G_{dd}^{0R\sigma}(\omega)$. So we can write down expression for $G_{dd}^{0R\sigma}(\omega)$:

$$\begin{aligned}G_{dd}^{0R\sigma}(\omega) &= \frac{1}{\omega - \varepsilon_d - \Sigma(\omega)} \\ \Sigma(\omega) &= \frac{n_{d-\sigma} U (\omega - \varepsilon_d)}{\omega - \varepsilon_d - (1 - n_{d-\sigma})U - i\delta} \end{aligned} \quad (5)$$

With the help of Keldysh diagram technique [14] using system of Dyson equations one can get expression for impurity retarded Green's function.

$$G_{dd}^{R\sigma} = \frac{1}{\omega - \varepsilon_d - \Sigma(\omega) - i(\gamma_{kd} + \gamma_{pd})} \quad (6)$$

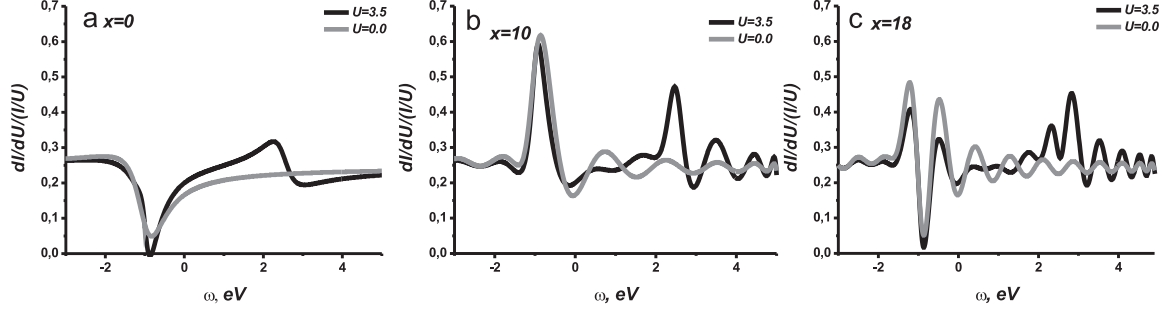


FIG. 2: Local tunneling conductivity as a function of applied bias voltage calculated for different values of the distance x from the deep impurity atom along the atomic chain in the absence (gray line) and in the presence (black line) of Coulomb interaction U . For all the figures values of the parameters $a = 1$, $t = 0,22$, $T = 0,18$, $\tau = 0,50$, $\Im = 1,00$, $\varepsilon_d = -1,00$, $U = 3,50$, $\nu_k^0 = 1$ are the same.

To evaluate the dependence of local tunneling conductivity on the distance from the deep impurity in the presence of Coulomb interaction expressions for $ImG_{dd}^R(\omega)$ and $ReG_{dd}^R(\omega)$ in formula 2 have to be retarded by expressions for $ImG_{dd}^{R\sigma}(\omega)$ and $ReG_{dd}^{R\sigma}(\omega)$. It is also necessary to take into account the presence of electron spin, it results in extra summation over σ and leads to additional factor equal to 2 in formula 2. Calculating expressions for $ImG_{dd}^{R\sigma}(\omega)$ and $ReG_{dd}^{R\sigma}(\omega)$ requires solution of self-consistent system of equations. Two of them are equations for $ImG_{dd}^{R\pm\sigma}(\omega)$, calculated from expression 6, and three equations determine impurity atom non-equilibrium electron filling numbers:

$$n_{d\mp\sigma} = \frac{-1}{\pi} \int d\omega n_{d\mp\sigma}(\omega) ImG_{dd}^{R\pm\sigma}(\omega, n_{d\pm\sigma})$$

$$n_{d\sigma}(\omega) = n_{d-\sigma}(\omega) = \frac{\gamma_{kd}n_k^0(\omega) + \gamma_{pd}n_p^0(\omega)}{\gamma_{kd} + \gamma_{pd}} \quad (7)$$

where $n_k^0(\omega)$ and $n_p^0(\omega)$ are equilibrium filling numbers in the tunneling contact leads.

Figure 2 shows tunneling conductivity as a function of applied bias voltage for different values of distance from the deep impurity. Tunneling conductivity calculated above the impurity has a resonant dip when applied bias voltage is equal to impurity energy level position ($\omega = \varepsilon_d$) both for taking (Fig. 2a black line) and not taking into account Coulomb interaction effects (Fig. 2a gray line). Tunneling conductivity calculated above the impurity in the presence of Coulomb interaction also reveals peak at the value of applied bias voltage equal to initial impurity energy level position shifted on the value of Coulomb potential ($\omega = \varepsilon_d + U$) in comparison with the case when Coulomb interaction effects are neglected.

At the fixed parameters of tunneling contact existence of a dip or a peak in tunneling conductivity in both resonances when applied bias voltage is equal to the impurity

energy levels positions is determined by the value of a distance.

It is clearly evident that in the case of deep impurity state Coulomb interaction effects lead to negligible shift of a resonant peculiarity which corresponds to value of applied bias voltage equal to initial impurity energy level position ($\omega = \varepsilon_d$). Suggested model also demonstrates absence of resonant peculiarities spreading with increasing of relaxation rates and distance value from the impurity.

Now let us analyze modification of formula 2 due to Coulomb interaction effects in the situation of shallow impurity state. In this case Coulomb interaction effects can be taken into account with the help of mean-field approximation (adopted parameters of the model correspond to the mixed valence regime). It means simply that impurity energy level position depends on Coulomb interaction of the non-equilibrium electron density. New impurity energy level position improved by Coulomb interaction can be found from the equation:

$$\tilde{\varepsilon}_d = \varepsilon_d + U \langle n_d \rangle \quad (8)$$

where ε_d is the initial position of impurity energy level without Coulomb interaction. Now the main point is that the non-equilibrium electron filling numbers n_d for impurity atom must satisfy self-consistency condition:

$$n_d = \frac{-1}{\pi} \int d\omega n_d(\omega) ImG_{dd}^R(\omega) \quad (9)$$

where $ImG_{dd}^R(\omega)$ is determined from equation 3 considering $\tilde{\varepsilon}_d$ substitution instead of ε_d . Impurity filling numbers $n_d(\omega)$ can be found from kinetic equations for Keldysh functions $G^<$ [7]:

$$n_d(\omega) = \frac{\gamma_{kd}n_k^0(\omega) + \gamma_{pd}n_p^0(\omega)}{\gamma_{kd} + \gamma_{pd}} \quad (10)$$

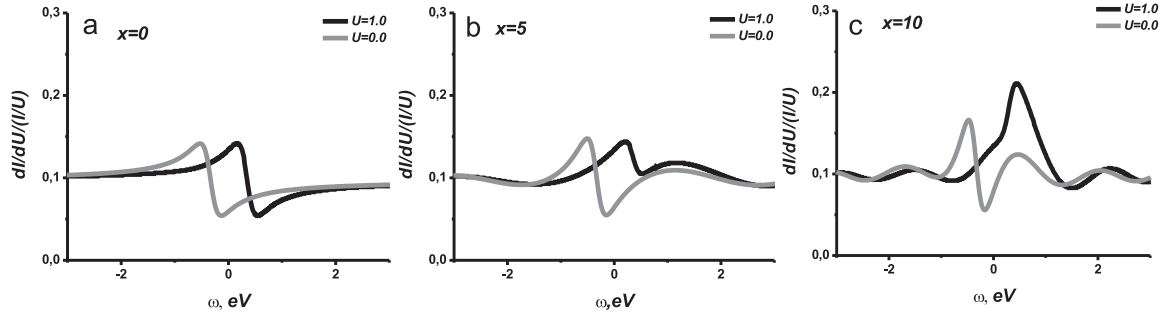


FIG. 3: Local tunneling conductivity as a function of applied bias voltage calculated for different values of the distance x from the shallow impurity atom along the atomic chain in the absence (gray line) and in the presence (black line) of Coulomb interaction U . For all the figures values of the parameters $a = 1$, $t = 0,22$, $T = 0,18$, $\tau = 0,40$, $\Im = 1,00$, $\varepsilon_d = -0,15$, $U = 1,00$, $\nu_k^0 = 1$ are the same.

After calculating impurity atom electron filling numbers n_d from the system of equations 3, 8-10 we can determine new position of impurity energy level $\tilde{\varepsilon}_d$. Next step in local tunneling conductivity calculation in the presence of Coulomb interaction for shallow impurities consists in replacement of energy level value ε_d by new value $\tilde{\varepsilon}_d$ in formula 2.

Figure 3 shows tunneling conductivity as a function of applied bias voltage for different values of distance from the shallow impurity. In this case tunneling conductivity calculated above the impurity has Fano line shape due to interference between resonant and non-resonant tunneling channels both for taking (black line) and not taking (gray line) into account Coulomb interaction effects (Fig. 3a). Tunneling conductivity calculated without Coulomb interaction (Fig. 3a gray line) shows a resonant dip when applied bias voltage is equal to impurity energy level position ($\omega = \varepsilon_d$). Considering Coulomb interaction for shallow impurities in the mean field approximation leads to a resonant dip shift to the higher values of applied bias voltage (Fig. 3a black line). This effect also takes place with increasing of the distance value from the impurity moreover shift is accompanied by dip's spreading (Fig. 3b black line). Dip's spreading is a result of both impurity initial energy level movement due to Coulomb interaction effects and increasing of relaxation rates in the studied system. It was found that dip's spreading is mostly significant when relaxation rate value exceeds value of initial impurity energy level position ε_d . Further increasing of distance (Fig. 3c black line) shows disappearing of the resonant dip in the case of Coulomb interaction opposing to the calculations carried out without taking into account Coulomb interaction effects (Fig.

3c gray line). Disappearing of a dip is a result of nearest to the dip peaks spreading (one of the peaks corresponds to the lower value of applied bias voltage and another to the higher value of applied bias voltage in comparison with dip position).

III. CONCLUSION

In this work we have analyzed the role of interplay effects between interference in tunneling processes and Coulomb interaction in spatial distribution of tunneling conductivity. We have studied two extreme cases when resonant tunneling takes place through deep impurity state and through shallow impurity state. In the case of deep impurity state non-equilibrium Coulomb interaction effects were analyzed with the help of Hubbard-I model. For shallow impurity state Coulomb interaction of localized electrons was treated self-consistently in the mean field approximation.

For shallow impurity state taking into account Coulomb interaction leads to the shift of a resonant dip to higher values of applied bias voltage and to the dip's spreading with increasing of tunneling relaxation rates values in comparison with the case of Coulomb interaction neglecting.

For deep impurity state taking into account Coulomb interaction results in formation of additional peculiarity which corresponds to the value of applied bias voltage equal to initial impurity energy level position shifted on the value of Coulomb potential.

This work was supported by RFBR grants and by the National Grants for technical regulation and metrology.

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